# Package 'DiffusionRgqd'

October 12, 2015

Title Inference and Analysis for Generalized Quadratic Diffusions

Version 0.1.0

<b>Description</b> Tools for performing inference and analysis on a class of quadratic diffusion processes for both scalar and bivariate diffusion systems. For scalar diffusions, a module is provided for solving first passage time problems for both time-homogeneous and time-inhomogeneous GQDs.
<pre>URL https://github.com/eta21</pre>
BugReports https://github.com/eta21/DiffusionRgqd/issues
MailingList Please send questions and comments to etiennead@gmail.com.
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DiffusionRgqd-package A package for Performing Inference and Analysis on Generalized Quadratic Diffusion Processes (GQDs).

## **Description**

**DiffusionRqqd** is a toolbox for performing analysis and inference on a class of diffusion processes with quadratic drift and diffusion. The package consists of functions for performing likelihood based inference and transitional density approximations for both 1D and 2D GQDs. For scalar diffusions, a module is provided for solving first passage time problems for both time homogeneous and time inhomogeneous GQDs.

#### **Details**

Package: DiffusionRgqd
Type: Package
Version: 0.0.0.9000
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License: GPL (>= 3)

The package is designed around an interface whereby the user supplies standard R-functions dictating the functional form of the coefficients of the GQD. For example, for scalar GQDs nested within the stochastic differential equation:

$$dX_t = (G_0(t) + G_1(t)X_t + G_2(t)X_t^2)dt + \sqrt{Q_0(t) + Q_1(t)X_t + Q_2(t)X_t^2}dW_t,$$

the user supplies GO(t),G1(t) and Q1(t) etc. These coefficients may depend on a both vector of parameters and time. The package handles all the necessary mathematics and algorithmic construction. Furthermore, computational efficiency is optimized by constructing algorithms in C++ using the **Rcpp** and **RcppArmadillo** libraries.

Functions included in the package:

BiGQD.density : Generate the transitional density of a 2D GQD.

BiGQD.mcmc\* : Conduct inference via MCMC on a 2D GQD.

BiGQD.mle\* : Calculate MLEs for a 2D GQD.

GQD.density : Generate the transitional density of a 1D GQD.

GQD.mcmc\* : Conduct inference via MCMC on a 1D GQD.

GQD.mle\* : Calculate MLEs for a 1D GQD.

GQD.passage\* : Approximate the first passage time density of a time homogeneous GQD to a barrier.

GQD.TIpassage\* : Approximate the first passage time density of a time-inhomogeneous GQD to a barrier.

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```
* Functions use C++.
```

#### Author(s)

```
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```

#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

#### See Also

```
BiGQD.mcmc, BiGQD.mle, GQD.mcmc, GQD.dic, GQD.mle,GQD.remove, GQD.passage, GQD.TIpassage and GQD.density.
```

# **Examples**

```
## Not run:
example(GQD.density)
example(BiGQD.density)
example(GQD.mcmc)
example(BiGQD.mcmc)
example(GQD.passage)
example(GQD.TIpassage)
## End(Not run)
```

BiGQD.density

Generate the Transition Density of a Bivariate Generalized Quadratic Diffusion Model (2D GQD).

# **Description**

BiGQD. density generates approximate transitional densities for bivariate generalized quadratic diffusions (GQDs). Given a starting coordinate, (Xs, Ys), the approximation is evaluated over a lattice  $Xt \times Yt$  for an equispaced discretization (intervals of width delt) of the transition time horizon [s, t].

# Usage

```
BiGQD.density(Xs, Ys, Xt, Yt, s, t, delt=1/100, Dtype='Saddlepoint')
```

# Arguments

Xt	x-Coordinates of the lattice at which to evaluate the transition density.
Yt	y-Coordinates of the lattice at which to evaluate the transition density.
Xs	Initial x-coordinate.
Ys	Initial y-coordinate.

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s Starting time of the diffusion.

t Final time at which to evaluate the transition density.

delt Step size for numerical solution of the cumulant system. Also used for the

discretization of the transition time-horizon. See warnings [1] and [2].

Dtype The density approximant to use. Valid types are "Saddlepoint" (default) or

"Edgeworth".

#### **Details**

BiGQD. density constructs an approximate transition density for a class of quadratic diffusion models. This is done by first evaluating the trajectory of the cumulants/moments of the diffusion numerically as the solution of a system of ordinary differential equations over a time horizon [s,t] split into equi-distant points delt units apart. Subsequently, the resulting cumulants/moments are carried into a density approximant (by default, a saddlepoint approximation) in order to evaluate the transtion surface.

#### Value

density 3D Array containing approximate density values. Note that the 3rd dimension

represents time.

Xmarginal 2D Array containing approximate Xt-marginal density values (calculated using

the univariate saddlepoint approximation).

Ymarginal 2D Array containing approximate Yt-marginal density values (calculated using

the univariate saddlepoint approximation).

Xt Copy of x-coordinates.
Yt Copy of y-coordinates.

time A vector containing the time mesh at which the density was evaluated.

cumulants A matrix giving the cumulants of the diffusion. Cumulants are indicated by

row-names.

# Warning

Warning [1]: The system of ODEs that dictate the evolution of the cumulants do so approximately. Thus, although it is unlikely such cases will be encountered in inferential contexts, it is worth checking (by simulation) whether cumulants accurately replicate those of the target GQD. Furthermore, it may in some cases occur that the cumulants are indeed accurate whilst the density approximation fails. This can again be verified by simulation.

**Warning** [2]: The parameter delt is also used as the stepsize for solving a system of ordinary differential equations (ODEs) that govern the evolution of the cumulants of the diffusion. As such delt is required to be small for highly non-linear models in order to ensure sufficient accuracy.

## Author(s)

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## References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

Daniels, H.E. 1954 Saddlepoint approximations in statistics. Ann. Math. Stat., 25:631–650.

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Eddelbuettel, D. and Romain, F. 2011 Rcpp: Seamless R and C++ integration. *Journal of Statistical Software*, **40**(8):1–18,. URL http://www.jstatsoft.org/v40/i08/.

Eddelbuettel, D. 2013 Seamless R and C++ Integration with Rcpp. New York: Springer. ISBN 978-1-4614-6867-7.

Eddelbuettel, D. and Sanderson, C. 2014 Repparmadillo: Accelerating R with high-performance C++ linear algebra. *Computational Statistics and Data Analysis*, **71**:1054–1063. URL http://dx.doi.org/10.1016/j.csda.2013.02.005.

Feagin, T. 2007 A tenth-order Runge-Kutta method with error estimate. *In Proceedings of the IAENG Conf. on Scientifc Computing*.

Varughese, M.M. 2013 Parameter estimation for multivariate diffusion systems. *Comput. Stat. Data An.*, **57**:417–428.

#### See Also

See BiGQD.mcmc and BiGQD.mle for likelihood based inference procedures for bivariate GQDs.

```
# Generate the transition density of a stochastic perturbed Lotka-Volterra
# preditor-prey model, with state-dependent volatility:
\# dX = (1.5X-0.4*X*Y)dt
                             +sqrt(0.05*X)dWt
\# dY = (-1.5Y+0.4*X*Y-0.2*Y^2)dt + sqrt(0.10*Y)dBt
# Remove any existing coefficients
GQD.remove()
# Define the X dimesnion coefficients
a10 = function(t)\{1.5\}
a11 = function(t)\{-0.4\}
c10 = function(t)\{0.05\}
# Define the Y dimension coefficients
b01 = function(t)\{-1.5\}
b11 = function(t)\{0.4\}
b02 = function(t)\{-0.2\}
f01 = function(t)\{0.1\}
# Approximate the transition density
res = BiGQD.density(5,5,seq(3,8,length=25),seq(2,6,length=25),0,10,1/100)
#-----
# Visuallize the density
par(ask=FALSE)
# Load simulated trajectory of the joint expectation:
data(SDEsim3)
attach(SDEsim3)
# We will simulate some trajectories (crudely) as well:
N=1000; delt= 1/100 # 1000 trajectories
```

```
X1=rep(5,N)
                     # Initial values for each trajectory
X2=rep(5,N)
for(i in 1:1001)
  # Applly Euler-Murayama scheme to the LV-model
  X1=pmax(X1+(a10(d)*X1+a11(d)*X1*X2)*delt+sqrt(c10(d)*X1)*rnorm(N,sd=sqrt(delt)),0)
 X2=pmax(X2+(b01(d)*X2+b11(d)*X1*X2+b02(d)*X2^2)*delt+sqrt(f01(d)*X2)*rnorm(N,sd=sqrt(delt)),0)
  # Now illustrate the density:
  filled.contour(res$Xt,res$Yt,res$density[,,i],
  main=paste0('Transition Density \n (t = ',res$time[i],')'),
  color.palette=colorRampPalette(c('white','green','blue','red'))
  ,xlab='Prey',ylab='Preditor',plot.axes=
     # Add simulated trajectories
     points(X2~X1,pch=20,col='grey47',cex=0.01)
     # Add trajectory of simulated expectation
     lines(my~mx,col='grey57')
     # Show the predicted expectation from BiGQD.density()
     points(res$cumulants[5,i]~res$cumulants[1,i],bg='white',pch=21,cex=1.5)
     axis(1);axis(2);
     # Add a legend
     legend('topright',lty=c('solid',NA,NA),col=c('grey57','grey47','black'),
             pch=c(NA,20,21),legend=c('Simulated Expectation','Simulated Trajectories'
             , 'Predicted Expectation'))
   })
}
```

BiGQD.mcmc

MCMC Inference on Bivariate Generalized Quadratic Diffusions (2D GQDs).

## Description

BiGQD.mcmc() uses parametrised coefficients (provided by the user as R-functions) to construct a C++ program in real time that allows the user to perform Bayesian inference on the resulting diffusion model. Given a set of starting parameters and other input parameters, a MCMC chain is returned for further analysis. The user may specify any model within the GQD framework by defining parametrised functions giving the form of the coefficients of the model. See the package manual for a description of the process.

#### Usage

#### **Arguments**

X A matrix containing rows of data points to be modelled. Although observations

are allowed to be non-equidistant, observations in both dimensions are assumed to occur at the same time epochs (i.e. time gives the time signature for both

dimensions).

time A vector containing the time epochs at which observations were made.

mesh The number of mesh points in the time discretization.

The parameter vector of the process. theta are taken as the starting values of the

MCMC chain and gives the dimension of the parameter vector used to calculate the DIC. Care should be taken to ensure that each element in theta is in fact used within the coefficient-functions, otherwise redundant parameters will be

counted in the calculation of the DIC.

sds Proposal distribution standard deviations. That is, for the i-th parameter the

proposal distribution is  $\sim Normal(..., sds[i]^2)$ .

updates The number of MCMC updates/iterations to perform (including burn-in).

burns The number of MCMC updates/iterations to burn.

exclude Vector indicating which transitions to exclude from the analysis. Default = NULL.

plot.chain If = TRUE (default), a trace plot of the MCMC chain will be made along with a

trace of the acceptance rate.

RK.order The order of the Runge-Kutta solver used to approximate the trajectories of

cumulants. Must be 4 (default) or 10.

Tag can be used to name (tag) an MCMC run e.g. Tag='Run\_1'

Dtype The density approximant to use. Valid types are "Saddlepoint" (default),

"Edgeworth" or "Normal".

recycle Whether or not to recycle the roots calculated for the saddlepoint approximation

over succesive updates.

rtf Starting vector for internal use.

wrt If TRUE a .cpp file will be written to the current directory. For bug report diag-

nostics.

#### Value

par.matrix A matrix containing the MCMC chain on theta.

acceptence.rate

A vector containing the acceptance rate of the MCMC at every iteration.

model.info A list of variables pertaining to inference calculations.

 ${\tt model.info\$elapsed.time}$ 

The runtime, in h/m/s format, of the MCMC procedure (excluding compile time).

model.info\$time.homogeneous

'No' if the model has time-homogeneous coefficients and 'Yes' otherwise.

model.info\$p The dimension of theta.

model.info\$DIC Calculated Deviance Information Criterion.

model.info\$pd Effective number of parameters (see model.info\$DIC).

#### Syntactical jargon

**Synt.** [1]: The coefficients of the 2D GQD may be parameterized using the reserved variable theta. For example:

```
a00 <- function(t){theta[1]*(theta[2]+sin(2*pi*(t-theta[3])))}.
```

**Synt.** [2]: Due to syntactical differences between R and C++ special functions have to be used when terms that depend on t. When the function cannot be separated in to terms that contain a single t, the prod(a,b) function must be used. For example:

```
a00 \leftarrow function(t)\{0.1*(10+0.2*sin(2*pi*t)+0.3*prod(sqrt(t),1+cos(3*pi*t)))\}.
```

Here sqrt(t)\*cos(3\*pi\*t) constitutes the product of two terms that cannot be written i.t.o. a single t. To circumvent this isue, one may use the prod(a,b) function.

**Synt.** [3]: Similarly, the  $^{\wedge}$  - operator is not overloaded in C++. Instead the pow(x,p) function may be used to calculate  $x^{p}$ . For example  $\sin(2*pi*t)^{3}$  in:

```
a00 <- function(t)\{0.1*(10+0.2*pow(sin(2*pi*t),3))\}.
```

#### Warning

Warning [1]: The parameter mesh is used to discretize the transition horizons between successive observations. It is thus important to ensure that mesh is not too small when large time differences are present in time. Check output for max(dt) and divide by mesh.

#### Note

**Note** [1]: When plot. chain is TRUE, a trace plot is created of the resulting MCMC along with the acceptance rate at each update. This may save time when scrutinizing initial MCMC runs.

# Author(s)

Etienne A.D. Pienaar <etiannead@gmail.com>

#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

Daniels, H.E. 1954 Saddlepoint approximations in statistics. *Ann. Math. Stat.*, **25**:631–650.

Eddelbuettel, D. and Romain, F. 2011 Rcpp: Seamless R and C++ integration. *Journal of Statistical Software*, **40**(8):1–18,. URL http://www.jstatsoft.org/v40/i08/.

Eddelbuettel, D. 2013 Seamless R and C++ Integration with Rcpp. New York: Springer. ISBN 978-1-4614-6867-7.

Eddelbuettel, D. and Sanderson, C. 2014 Repparmadillo: Accelerating R with high-performance C++ linear algebra. *Computational Statistics and Data Analysis*, **71**:1054–1063. URL http://dx.doi.org/10.1016/j.csda.2013.02.005.

Feagin, T. 2007 A tenth-order Runge-Kutta method with error estimate. *In Proceedings of the IAENG Conf. on Scientifc Computing*.

Varughese, M.M. 2013 Parameter estimation for multivariate diffusion systems. *Comput. Stat. Data An.*, **57**:417–428.

# See Also

```
GQD.remove, BiGQD.mle, GQD.mcmc, GQD.mle, GQD.passage and GQD.TIpassage.
```

```
# This example simulates a bivariat time homogeneous diffusion and shows how
# to conduct inference using BiGQD.mcmc(). We fit two competing models and then
# use the output to select a winner.
  data(SDEsim2)
  data(SDEsim2)
  attach(SDEsim2)
  # Have a look at the time series:
 plot(Xt~time,type='1',col='blue',ylim=c(2,10),main='Simulated Data',xlab='Time (t)',ylab='State',
       axes=FALSE)
  lines(Yt~time,col='red')
  expr1=expression(dX[t]==2(Y[t]-X[t])*dt+0.3*sqrt(X[t]*Y[t])*dW[t])
  expr2=expression(dX[t]==(5-Y[t])*dt+0.5*sqrt(Y[t])*dB[t])
  text(50,9,expr1)
  text(50,8.5,expr2)
  axis(1, seq(0, 100, 5))
  axis(1, seq(0, 100, 5/10), tcl=-0.2, labels=NA)
  axis(2, seq(0, 20, 2))
  axis(2, seq(0, 20, 2/10), tcl=-0.2, labels=NA)
 # Define the coefficients of a proposed model
 GQD.remove()
  a00 <- function(t){theta[1]*theta[2]}</pre>
  a10 <- function(t){-theta[1]}</pre>
  c00 <- function(t){theta[3]*theta[3]}</pre>
  b00 <- function(t){theta[4]}</pre>
  b01 <- function(t){-theta[5]}</pre>
  f00 <- function(t){theta[6]*theta[6]}</pre>
  theta.start <- c(3,3,3,3,3,3)
  prop.sds <-c(0.15,0.16,0.04,0.99,0.19,0.04)
             <- 50000
  updates
              <- cbind(Xt,Yt)
  # Define prior distributions:
  priors=function(theta){dunif(theta[1],0,100)*dunif(theta[4],0,100)}
  # Run the MCMC procedure
  m1=BiGQD.mcmc(X,time,10,theta.start,prop.sds,updates)
 # Remove old coefficients and define the coefficients of a new model
 GQD.remove()
  a10 <- function(t){-theta[1]}</pre>
  a01 <- function(t){theta[1]*theta[2]}</pre>
 c11 <- function(t){theta[3]*theta[3]}</pre>
  b00 <- function(t){theta[4]*theta[5]}</pre>
```

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BiGQD.mle

Calculate Maximum Likelihood Estimates for a 2D GQD Model.

# Description

BiGQD.mle() uses parametrised coefficients (provided by the user as R-functions) to construct a C++ program in real time that allows the user to perform maximum likelihood inference on the resulting diffusion model. The user may specify any model within the GQD framework by defining parametrised functions giving the form of the coefficients of the model. See the package manual for a description of the process.

# Usage

# Arguments

X	A matrix containing rows of data points to be modelled. Though observations are allowed to be non-equidistant, observations in both dimensions are assumed to occur at the same time epochs.
time	A vector containing the time epochs at which observations were made.
mesh	The number of mesh points in the time discretisation.
theta	The parameter vector starting values.
control	List of control variables to be used by optim.

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method Method to be used by optim. Vector indicating which transitions to exclude from the analysis. Default = NULL. exclude RK.order The order of the Runge-Kutta solver used to approximate the trajectories of cumulants. Must be 4 (default) or 10. Tag can be used to name (tag) an MCMC run e.g. Tag='Run\_1' Tag The density approximant to use. Valid types are "Saddlepoint" (default), Dtype "Edgeworth" or "Normal". Starting vector for internal use. rtf wrt

If TRUE a .cpp file will be written to the current directory. For bug report diag-

#### Value

The output from optim. opt model.info A list of variables pertaining to inference calculations. model.info\$elapsed.time The runtime, in h/m/s format, of the MCMC procedure (excluding compile time).  ${\tt model.info\$time.homogeneous}$ 'No' if the model has time-homogeneous coefficients and 'Yes' otherwise.

The dimension of theta.

# Syntactical jargon

model.info\$p

Synt. [1]: The coefficients of the 2D GQD may be parameterized using the reserved variable theta. For example:

```
a00 <- function(t){theta[1]*(theta[2]+sin(2*pi*(t-theta[3])))}.
```

Synt. [2]: Due to syntactical differences between R and C++ special functions have to be used when terms that depend on t. When the function cannot be separated in to terms that contain a single t, the prod(a,b) function must be used. For example:

```
a00 \leftarrow function(t) \{0.1*(10+0.2*sin(2*pi*t)+0.3*prod(sqrt(t),1+cos(3*pi*t)))\}.
```

Here sqrt(t)\*cos(3\*pi\*t) constitutes the product of two terms that cannot be written i.t.o. a single t. To circumvent this isue, one may use the prod(a,b) function.

Synt. [3]: Similarly, the  $^{\wedge}$  - operator is not overloaded in C++. Instead the pow(x,p) function may be used to calculate  $x^p$ . For example  $\sin(2*pi*t)^3$  in:

```
a00 \leftarrow function(t)\{0.1*(10+0.2*pow(sin(2*pi*t),3))\}.
```

# Warning

Warning [1]: The parameter mesh is used to discretize the transition horizons between successive observations. It is thus important to ensure that mesh is not too small when large time differences are present in time. Check output for max(dt) and divide by mesh.

Warning [2]: Note that minus the likelihood is minimized, as such the optim output (hessian) needs to be adjusted accordingly if used for calculating confidence intervals. Furthermore, GQD.mle may be temperamental under certain conditions

## Author(s)

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#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

Daniels, H.E. 1954 Saddlepoint approximations in statistics. Ann. Math. Stat., 25:631–650.

Eddelbuettel, D. and Romain, F. 2011 Rcpp: Seamless R and C++ integration. *Journal of Statistical Software*, **40**(8):1–18,. URL http://www.jstatsoft.org/v40/i08/.

Eddelbuettel, D. 2013 *Seamless R and C++ Integration with Rcpp*. New York: Springer. ISBN 978-1-4614-6867-7.

Eddelbuettel, D. and Sanderson, C. 2014 Repparmadillo: Accelerating R with high-performance C++ linear algebra. *Computational Statistics and Data Analysis*, **71**:1054–1063. URL http://dx.doi.org/10.1016/j.csda.2013.02.005.

Feagin, T. 2007 A tenth-order Runge-Kutta method with error estimate. *In Proceedings of the IAENG Conf. on Scientifc Computing*.

Varughese, M.M. 2013 Parameter estimation for multivariate diffusion systems. *Comput. Stat. Data An.*, **57**:417–428.

# See Also

```
GQD.remove, BiGQD.mcmc, GQD.mcmc, GQD.mle, GQD.passage and GQD.TIpassage.
```

```
# This example simulates a bivariate time homogeneous diffusion and shows how
# to conduct inference using BiGQD.mle(). We fit two competing models and then
# use the output to select a winner.
 data(SDEsim2)
 data(SDEsim2)
 attach(SDEsim2)
 # Have a look at the time series:
 plot(Xt~time,type='1',col='blue',ylim=c(2,10),main='Simulated Data',xlab='Time (t)',ylab='State',
      axes=FALSE)
 lines(Yt~time,col='red')
 expr1=expression(dX[t]==2(Y[t]-X[t])*dt+0.3*sqrt(X[t]*Y[t])*dW[t])
 \label{eq:continuous} {\sf expr2=expression(dX[t]==(5-Y[t])*dt+0.5*sqrt(Y[t])*dB[t])}
 text(50.9.expr1)
 text(50,8.5,expr2)
 axis(1, seq(0, 100, 5))
 axis(1, seq(0, 100, 5/10), tcl=-0.2, labels=NA)
 axis(2, seq(0, 20, 2))
 axis(2, seq(0, 20, 2/10), tcl=-0.2, labels=NA)
 # Define the coefficients of a proposed model
 GOD.remove()
 a00 <- function(t){theta[1]*theta[2]}</pre>
 a10 <- function(t){-theta[1]}
 c00 <- function(t){theta[3]*theta[3]}</pre>
```

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```
b00 <- function(t){theta[4]}</pre>
 b01 <- function(t){-theta[5]}</pre>
 f00 <- function(t){theta[6]*theta[6]}</pre>
 theta.start <- c(3,3,3,3,3,3)
         <- cbind(Xt,Yt)
 # Calculate MLEs
 m1=BiGQD.mle(X,time,10,theta.start)
#-----
# Remove old coefficients and define the coefficients of a new model
#-----
 GQD.remove()
 a10 <- function(t){-theta[1]}
 a01 <- function(t){theta[1]*theta[2]}</pre>
 c11 <- function(t){theta[3]*theta[3]}</pre>
 b00 <- function(t){theta[4]*theta[5]}</pre>
 b01 <- function(t){-theta[4]}</pre>
 f01 <- function(t){theta[6]*theta[6]}</pre>
 theta.start <- c(3,3,3,3,3,3)
 # Calculate MLEs
 m2=BiGQD.mle(X,time,10,theta.start)
# Compare estimates:
 GOD.estimates(m1)
 GQD.estimates(m2)
#-----
# Compare the two models
#-----
 GQD.aic(list(m1,m2))
```

GQD.aic

Summarize MLE Selection Output for a List of GQD.mle or BiGQD.mle objects.

# Description

GQD.aic() summarizes the MCMC output from a list of GQD.mle() objects. This may be used to neatly summarize the MCMC output of various models fitted to a given dataset.

# Usage

```
GQD.aic(model.list, type = "col")
```

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#### **Arguments**

```
model.list A list of GQD.mle() objects.

type Shoould output be of row ('row') or column ('col') format.
```

#### **Details**

GQD.aic() summarizes the output from various models fitted via GQD.mle(). By ranking them according to DIC. [=] indicates which model has the minimal DIC.

	Convergence	р	min.likelihood	AIC	BIC	N
Model 1	0	5	171.5576	[=] 353.1152	[=] 369.6317	201
Model 2	0	5	185.7518	381.5036	398.0201	201

#### Value

A data frame with summary of model output. See Details.

#### Author(s)

```
Etienne A.D. Pienaar: <etiannead@gmail.com>
```

#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

# See Also

GQD.mle

```
# Simulate a time inhomogeneous diffusion.
 data(SDEsim1)
 attach(SDEsim1)
 par(mfrow=c(1,1))
 expr1=expression(dX[t]==2*X[t]*(5+3*sin(0.5*pi*t)-X[t])*dt+0.5*X[t]*dW[t])
 plot(Xt^*time,type='l',col='blue',xlab='Time~(t)',ylab=expression(X[t]),main=expr1)
#-----
# Define coefficients of the process.
#-----
 GQD.remove()
 G0 <- function(t){theta[1]*(theta[2]+theta[3]*sin(0.25*pi*t))}
 G1 <- function(t){-theta[1]}</pre>
 Q0 <- function(t){theta[4]*theta[4]}
 theta.start <- c(1,1,1,1)
                                    # Starting values for the chain
 mesh.points <- 10
                                    # Number of mesh points
```

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GQD.density

Generate the Transition Density of a Scalar Generalized Quadratic Diffusion (GQD).

# Description

GQD. density approximates the transition density of a scalar generalized quadratic diffusion model (GQD). Given an initial value for the diffusion, Xs, the approximation is evaluated for all Xt at equispaced time-nodes given by splitting [s, t] into subintervals of length delt.

# Usage

```
GQD.density(Xs, Xt, s, t, delt=1/100, Dtype='Saddlepoint', Trunc=c(4,4), P=100, alpha=0, lower=0, upper=50)
```

# Arguments

Xs	Initial value of the process at time s.
Xt	Vector of values at which the transition density is to be evaluated over the trajectory of the transition density from time s to t.
S	The starting time of the process.
t	The time horizon up to and including which the transitional density is evaluated.
delt	Size of the time increments at which successive evaluations are made.
Dtype	Character string indicating the type of density approximation (see details) to use. Types: 'Saddlepoint', 'Normal', 'Gamma', 'InvGamma' and 'Beta' are supported (default = 'Saddlepoint').

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Trunc Vector of length 2 containing the cumulant truncation order and the density trun-

cation order respectively. May take on values 4, 6 and 8 with the constraint that

Trunc[1] >= Trunc[2]. Default is c(4,4).

P Normalization parameter indicating the number of points to use when normaliz-

ing members of the Pearson system (see details)

alpha Normalization parameter controlig the mesh concentration when normalizing

members of the Pearson system (see details). Increasing alpha decreases con-

centration around the mean and vice versa (default alpha = 0).

lower, upper Lower and upper bounds for the normalization range.

#### **Details**

GQD. density constructs an approximate transition density for a class of quadratic diffusion models. This is done by first evaluating the trajectory of the cumulants/moments of the diffusion numerically as the solution of a system of ordinary differential equations over a time horizon [s,t] split into equi-distant points delt units apart. Subsequently, the resulting cumulants/moments are carried into a density approximant (by default, a saddlepoint approximation) in order to evaluate the transtion surface.

#### Value

density A matrix giving the density over the spatio-temporal mesh whose vertices are

defined by paired permutations of the elements of X\_t and time

Xt A vector of points defining the state space at which the density was evalu-

ated(recycled from input).

time A vector of time points at which the density was evaluated.

cumulants A matrix giving the cumulants of the diffusion. Row i gives the i-th cumulant.

moments A matrix giving the moments of the diffusion. Row i gives the i-th cumulant.

mesh A matrix giving the mesh used for normalization of the density.

#### Warning

Warning [1]: The system of ODEs that dictate the evolution of the cumulants do so approximately. Thus, although it is unlikely such cases will be encountered in inferential contexts, it is worth checking (by simulation) whether cumulants accurately replicate those of the target GQD. Furthermore, it may in some cases occur that the cumulants are indeed accurate whilst the density approximation fails. This can again be verified by simulation after which alternate density approximants may be specified through the variable Dtype.

**Warning [2]**: The parameter delt is also used as the stepsize for solving a system of ordinary differential equations (ODEs) that govern the evolution of the cumulants of the diffusion. As such delt is required to be small for highly non-linear models in order to ensure sufficient accuracy.

#### Author(s)

Etienne A.D. Pienaar: <etiannead@gmail.com>

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#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

Daniels, H.E. 1954 Saddlepoint approximations in statistics. Ann. Math. Stat., 25:631-650.

Feagin, T. 2007 A tenth-order Runge-Kutta method with error estimate. *In Proceedings of the IAENG Conf. on Scientifc Computing*.

Varughese, M.M. 2013 Parameter estimation for multivariate diffusion systems. *Comput. Stat. Data An.*, **57**:417–428.

#### See Also

See GQD.mcmc and GQD.mle for likelihood based inference procedures for GQDs.

```
# Generate the transition density of a CIR process with time dependant
# drift and volatility.
 # Remove any existing coefficients
 GQD.remove()
 # Define drift Coefficients. Note that the limiting mean is sinusoidal.
 G0 \leftarrow function(t)\{2*(10+sin(2*pi*(t-0.5)))\}
 G1 \leftarrow function(t)\{-2\}
 # Define sinusoidal diffusion coefficient with `faster' oscillation.
 Q1 \leftarrow function(t)\{0.25*(1+0.75*(sin(4*pi*t)))\}
           <- seq(5,15,1/10) # State values
 states
 initial <- 8
                          # Starting value of the process
 Tmax
          <- 5
                          # Time horizon
          <- 1
 Tstart
                           # Time starts at 1
 increment <- 1/100
                           # Incremental time steps
 # Generate the transitional density
 M <- GQD.density(Xs=initial, Xt=states, s=Tstart, t=Tmax, delt=increment)
 if(require(rgl, quietly = TRUE))
   open3d(windowRect=c(50,50,640+50,50+640),zoom=0.95)
   persp3d(x=M$Xt,y=M$time,z=M$density,col=3,box=FALSE,xlab='State (X_t)',
          ylab='Time (t)',zlab='Density f(X_t|X_s)')
   play3d(spin3d(axis=c(0,0,1), rpm=3), duration=10)
 }else
   persp(x=M\$Xt,y=M\$time,z=M\$density,col=3,xlab='State~(X_t)',ylab='Time~(t)',
        zlab='Density f(X_t|X_s)',border=NA,shade=0.5,theta=145)
 }
# Generate the transition density for a diffusion process with restricted domain.
\# The diffusion has reflective boundaries at 0 and 1.
```

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\_\_\_\_\_\_

```
GQD.remove()
G0 \leftarrow function(t)\{0.4*(0.5+sin(2*pi*t))\}
G1 \leftarrow function(t)\{-0.4\}
Q1 <- function(t)\{0.25\}
Q2 \leftarrow function(t)\{-0.25\}
           <- seq(0.005,0.995,1/200)
states
initial
           <- 0.5
Tmax
           <- 5
increment <- 1/50
# Generate the transitional density
M <- GQD.density(Xs=initial, Xt=states, s=0, t=Tmax, delt=increment,
                 Dtype='Beta',Trunc=c(8,8))
if(require(rgl, quietly = TRUE))
 open3d(windowRect=c(50,50,640+50,50+640),zoom=0.95)
 persp3d(x=M$Xt,y=M$time,z=M$density,col='steelblue',box=FALSE,
          xlab='State (X_t)',ylab='Time (t)',zlab='Density f(X_t|X_s)')
 play3d(spin3d(axis=c(0,0,1), rpm=3), duration=10)
}else
 persp(x=M$Xt,y=M$time,z=M$density,col=3,xlab='State (X_t)',ylab='Time (t)',
        zlab='Density f(X_t|X_s)',border=NA,shade=0.5,theta=145)
}
```

GQD.dic

Summarize MCMC Selection Output for a List of GQD.mcmc or BiGQD.mcmc objects.

# **Description**

 $\protect\operatorname{GQD.dic}()$  summarizes the MCMC output from a list of  $\protect\operatorname{GQD.mcmc}()$  objects. This may be used to neatly summarize the MCMC output of various models fitted to a given dataset.

# Usage

```
GQD.dic(model.list, type = "col")
```

#### **Arguments**

```
model.list A list of GQD.mcmc() objects.

type Shoould output be of row ('row') or column ('col') format.
```

# Details

GQD.dic() summarizes the output from various models fitted via GQD.mcmc(). By ranking them according to DIC. [=] indicates which model has the minimal DIC.

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	Elapsed_Time	Time_Homogeneous	р	DIC	рD	N
Model 1	00:00:47	No	5.00	389.30	3.92	201
Model 2	00:01:00	No	5.00	[=]386.45	4.13	201
Model 3	00:02:50	No	5.00	391.37	3.94	201

#### Value

A data frame with summary of model output. See Details.

#### Author(s)

Etienne A.D. Pienaar: <etiannead@gmail.com>

#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

#### See Also

GQD.mcmc

```
# Simulate a time inhomogeneous diffusion.
data(SDEsim1)
attach(SDEsim1)
par(mfrow=c(1,1))
expr1=expression(dX[t]==2*X[t]*(5+3*sin(0.5*pi*t)-X[t])*dt+0.5*X[t]*dW[t])
plot(Xt~time,type='l',col='blue',xlab='Time (t)',ylab=expression(X[t]),main=expr1)
 #-----
 # Define coefficients of model 1
 # Remove any existing coefficents. If none are pressent NAs will be returned, but
 # this is a safeguard against overlapping.
   GQD.remove()
 # Define time dependant coefficients. Note that all functions have a single argument.
 # This argument has to be `t' in order for the dependancy to be recognized.
 # theta does not have to be defined as an argument.
 G0 \leftarrow function(t)\{theta[1]*(theta[2]+theta[3]*sin(0.25*pi*t))\}
 G1 <- function(t){-theta[1]}</pre>
 Q0 <- function(t){theta[4]*theta[4]}
 theta.start <- c(1,1,1,1)
                                           # Starting values for the chain
 proposal.sds \leftarrow c(0.8,0.1,0.1,0.1) # Std devs for proposal distributions
 mesh.points <- 10
                                            # Number of mesh points
```

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```
updates
             <- 50000
                                           # Perform 50000 updates
 priors=function(theta){dnorm(theta[1],5,5)}
 m1 <- GQD.mcmc(Xt,time,mesh=mesh.points,theta=theta.start,sds=proposal.sds,</pre>
              updates=updates)
# Define coefficients of model 2
#-----
 GQD.remove()
 G0 <- function(t){theta[1]*(theta[2]+theta[3]*sin(0.25*pi*t))}</pre>
 G1 <- function(t){-theta[1]}</pre>
 Q1 <- function(t){theta[4]*theta[4]}
 proposal.sds <- c(0.8,0.1,0.1,0.1)
 m2 <- GQD.mcmc(Xt,time,mesh=mesh.points,theta=theta.start,sds=proposal.sds,</pre>
              updates=updates)
#-----
# Define coefficients of model 3
 GQD.remove()
 G1 \leftarrow function(t)\{theta[1]*(theta[2]+theta[3]*sin(0.25*pi*t))\}
 G2 <- function(t){-theta[1]}</pre>
 Q2 <- function(t){theta[4]*theta[4]}
 proposal.sds = c(0.1, 0.1, 0.1, 0.05)
 m3 <- GQD.mcmc(Xt,time,mesh=mesh.points,theta=theta.start,sds=proposal.sds,
              updates=updates)
 # Checkthe parameter estimates:
 GQD.estimates(m3, thin = 200)
# Summarize the output from all three models.
GQD.dic(list(m1,m2,m3))
#-----
```

 ${\tt GQD.estimates}$ 

Extract Parmaeter Estimates from .mle() or .mcmc() Objects.

# Description

 ${\tt GQD.estimates()} \ calculates \ parameter \ estimates \ from \ .mle() \ or \ .mcmc() \ model \ objects.$ 

## Usage

```
GQD.estimates(x, thin = 100, burns)
```

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#### **Arguments**

x List object of type 'GQD.mcmc' or 'GQD.mle'. That is, when model =GQD.mcmc()

then model constitutes an appropriate object for x.

thin Thinnging level for parameter chain.

burns Number of MCMC updates to discard before calculating estimates.

#### Value

Data frame with parameter estimates and appropriate interval statistics.

#### Author(s)

```
Etienne A.D. Pienaar: <etiannead@gmail.com>
```

#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

#### See Also

```
GQD.mcmc, GQD.mle, BiGQD.mcmc and BiGQD.mle.
```

```
# This example simulates a time inhomogeneous diffusion and shows how to conduct
# inference using GQD.mcmc
                     -----
library(DiffusionRgqd)
data(SDEsim1)
par(mfrow=c(1,1))
x <- SDEsim1
plot(x$Xt~x$time,type='l',col='blue')
#-----
# Define parameterized coefficients of the process, and set up starting
# parameters.
# True model: dX_t = 2X_t(5+3\sin(0.25 \text{ pi t})-X_t)dt+0.5X_tdW_t
# Remove any existing coefficents. If none are pressent NAs will be returned, but
# this is a safeguard against overlapping.
GQD.remove()
# Define time dependant coefficients. Note that all functions have a single argument.
# This argument has to be `t' in order for the dependancy to be recognized.
# theta does not have to be defined as an argument.
G1 \leftarrow function(t)\{theta[1]*(theta[2]+theta[3]*sin(0.25*pi*t))\}
G2 <- function(t){-theta[1]}</pre>
Q2 <- function(t){theta[4]*theta[4]}
theta.start <-c(1,1,1,1)
                                      # Starting values for the chain
proposal.sds <- c(0.4,0.3,0.2,0.1)*1/2
                                    # Std devs for proposal distributions
```

GQD.mcmc

GQD.mcmc

MCMC Inference on Generalized Quadratic Diffusion Models (GQDs).

# **Description**

GQD.mcmc() uses parametrised coefficients (provided by the user as R-functions) to construct a C++ program in real time that allows the user to perform Bayesian inference on the resulting diffusion model. Given a set of starting parameters and other input parameters, a MCMC chain is returned for further analysis. The structure of the model is predefined and coefficients may be provided for models nested within the generalized quadratic diffusion framework. That is, the saturated GQD model is given by:

$$dX_t = (G_0(t) + G_1(t)X_t + G_2(t)X_t^2)dt + \sqrt{Q_0(t) + Q_1(t)X_t + Q_2(t)X_t^2}dW_t$$

where dW\_t is Standard Brownian Motion.

# Usage

#### **Arguments**

X	Time series (vector) of discretely observed points of the process of interest. These may be non-equidistant observations (see time).
time	A vector of time-stamps associated with each observation in X.
mesh	The number mesh points between any two given data points.
theta	The parameter vector of the process. theta are taken as the starting values of the MCMC chain and gives the dimension of the parameter vector used to calculate the DIC. Care should be taken to ensure that each element in theta is in fact used within the coefficient-functions, otherwise redundant parameters will be counted in the calculation of the DIC.

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sds	Proposal distribution standard deviations. That is, for the i-th parameter the proposal distribution is $\sim Normal(, sds[i]^2)$
updates	The number of chain updates (including burned updates) to perform.
burns	The number of updates to burn. That is, the first burns values are omitted from the inference, although the entire chain is returned.
exclude	Vector indicating which transitions to exclude from the analysis. Default = NULL.
plot.chain	If TRUE (default), a trace plot is made of the resulting MCMC chain (see details).
RK.order	The order of the Runge-Kutta solver used to approximate the trajectories of cumulants. Must be 4 or (default) 10.
Dtype	Character string indicating the type of density approximation (see details) to use. Types: 'Saddlepoint', 'Normal', 'Gamma', 'InvGamma' and 'Beta' are supported (default = 'Saddlepoint').
Trunc	Vector of length 2 containing the cumulant truncation order and the density truncation order respectively. May take on values 4, 6 and 8 with the constraint that Trunc[1] >= Trunc[2]. Default is c(4,4).
P	Normalization parameter indicating the number of points to use when normalizing members of the Pearson system (see details)
alpha	Normalization parameter controlig the mesh concentration when normalizing members of the Pearson system (see details). Increasing alpha decreases concentration around the mean and vice versa (default alpha = $0$ ).
lower,upper	Lower and upper bounds for the normalization range.
Tag	Tag can be used to name (tag) an MCMC run e.g. Tag='Run_1'
wrt	If TRUE a .cpp file will be written to the current directory. For bug report diagnostics.

## **Details**

GQD.mcmc() operates by searching the workspace for functions with names that match the coefficients of the predefined stochastic differential equation. Only the required coefficients need to be specified e.g. GO(t),GI(t) and GO(t) for an Ornstein-Uhlenbeck model. Unspecified coefficients are ignored. When a new model is to be defined, the current model may be removed from the workspace by using the GQD.remove function, after which the new coefficients may be supplied.

## Value

par.matrix A matrix containing the MCMC chain on theta.

acceptence.rate

A vector containing the acceptance rate of the MCMC at every iteration.

model.info A list of variables pertaining to inference calculations.

model.info\$elapsed.time

The runtime, in h/m/s format,of the MCMC procedure (excluding compile time).

model.info\$time.homogeneous

'No' if the model has time-homogeneous coefficients and 'Yes' otherwise.

model.info\$p The dimension of theta.

model.info\$DIC Calculated Deviance Information Criterion.

model.info\$pd Effective number of parameters (see model.info\$DIC).

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#### Syntactical jargon

**Synt.** [1]: The coefficients of the 2D GQD may be parameterized using the reserved variable theta. For example:

```
G0 <- function(t){theta[1]*(theta[2]+sin(2*pi*(t-theta[3])))}.
```

**Synt.** [2]: Due to syntactical differences between R and C++ special functions have to be used when terms that depend on t. When the function cannot be separated in to terms that contain a single t, the prod(a,b) function must be used. For example:

```
G0 \leftarrow function(t)\{0.1*(10+0.2*sin(2*pi*t)+0.3*prod(sqrt(t),1+cos(3*pi*t)))\}.
```

Here sqrt(t)\*cos(3\*pi\*t) constitutes the product of two terms that cannot be written i.t.o. a single t. To circumvent this isue, one may use the prod(a,b) function.

**Synt.** [3]: Similarly, the  $^{\land}$  - operator is not overloaded in C++. Instead the pow(x,p) function may be used to calculate  $x^{\land}p$ . For example  $\sin(2*pi*t)^{\land}3$  in:

```
G0 <- function(t)\{0.1*(10+0.2*pow(sin(2*pi*t),3))\}.
```

#### Note

**Note** [1]: When plot. chain is TRUE, a trace plot is created of the resulting MCMC along with the acceptance rate at each update. This may save time when scrutinizing initial MCMC runs.

## Author(s)

Etienne A.D. Pienaar: <etiennead@gmail.com>

#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

Daniels, H.E. 1954 Saddlepoint approximations in statistics. Ann. Math. Stat., 25:631–650.

Eddelbuettel, D. and Romain, F. 2011 Rcpp: Seamless R and C++ integration. *Journal of Statistical Software*, **40**(8):1–18,. URL http://www.jstatsoft.org/v40/i08/.

Eddelbuettel, D. 2013 *Seamless R and C++ Integration with Rcpp*. New York: Springer. ISBN 978-1-4614-6867-7.

Eddelbuettel, D. and Sanderson, C. 2014 Repparmadillo: Accelerating R with high-performance C++ linear algebra. *Computational Statistics and Data Analysis*, **71**:1054–1063. URL http://dx.doi.org/10.1016/j.csda.2013.02.005.

Feagin, T. 2007 A tenth-order Runge-Kutta method with error estimate. *In Proceedings of the IAENG Conf. on Scientifc Computing*.

Varughese, M.M. 2013 Parameter estimation for multivariate diffusion systems. *Comput. Stat. Data An.*, **57**:417–428.

#### See Also

```
GQD.remove, GQD.mle, BiGQD.mcmc, BiGQD.mle, GQD.passage and GQD.TIpassage.
```

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#### **Examples**

```
# This example simulates a time inhomogeneous diffusion and shows how to conduct
# inference using GQD.mcmc
 data(SDEsim1)
 attach(SDEsim1)
 par(mfrow=c(1,1))
 \texttt{expr1} = \texttt{expression}(\texttt{dX[t]} = 2 \times \texttt{X[t]} \times (5 + 3 \times \sin(0.5 \times \text{pi} \times \text{t}) - \texttt{X[t]}) \times \texttt{dt} + 0.5 \times \texttt{X[t]} \times \texttt{dW[t]})
plot(Xt^*time, type='l', col='blue', xlab='Time\ (t)', ylab=expression(X[t]), main=expr1)
#-----
# Define parameterized coefficients of the process, and set up starting
# parameters.
# True model: dX_t = 2X_t(5+3\sin(0.25 \text{ pi t})-X_t)dt+0.5X_tdW_t
# Remove any existing coefficents. If none are pressent NAs will be returned, but
# this is a safeguard against overlapping.
GQD.remove()
# Define time dependant coefficients. Note that all functions have a single argument.
# This argument has to be `t' in order for the dependancy to be recognized.
# theta does not have to be defined as an argument.
G1 <- function(t){theta[1]*(theta[2]+theta[3]*sin(0.25*pi*t))}</pre>
G2 <- function(t){-theta[1]}</pre>
Q2 <- function(t){theta[4]*theta[4]}
theta.start <-c(1,1,1,1)
                                                  # Starting values for the chain
proposal.sds <- c(0.4,0.3,0.2,0.1)*1/2
                                                 # Std devs for proposal distributions
mesh.points <- 10
                                                  # Number of mesh points
              <- 50000
updates
                                                  # Perform 50000 updates
# Run the MCMC procedure for the model defined above
m1 <- GQD.mcmc(Xt,time,mesh=mesh.points,theta=theta.start,sds=proposal.sds,</pre>
                updates=updates,RK.order=4,wrt=T)
# Calculate estimates:
GQD.estimates(m1,thin=200)
```

GQD.mle

MLEs for Generalized Quadratic Diffusion Models (GQDs).

# **Description**

GQD.mle() constructs a C++ program in real time that allows the user to perform maximum likelihood inference on scalar GQDs. Given a set of starting parameters, the maximum likelihood estimates are calculated via minimization of minus the likelihood function via the built-in R-function

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optim. The structure of the model is predefined and coefficients may be provided for models nested within the generalized quadratic diffusion framework. That is, the saturated GQD model is given by:

$$dX_t = (G_0(t) + G_1(t)X_t + G_2(t)X_t^2)dt + \sqrt{Q_0(t) + Q_1(t)X_t + Q_2(t)X_t^2}dW_t$$

where dW t is Standard Brownian Motion.

#### Usage

## **Arguments**

X Time series (vector) of discretely observed points of the process of interest.
These may be non-equidistant observations (see time).

time A vector of time-stamps associated with each observation in X.

mesh The number mesh points between any two given data points.

The number mesh points between any two given data points.

The set of starting parameters for the optimization routine.

control List of control variables to be used by optim.

method Method to be used by optim.

exclude Vector indicating which transitions to exclude from the analysis. Default = NULL.

RK.order The order of the Runge-Kutta scheme used. Value must be 4 or (default) 10.

Dtype Character string indicating the type of density approximation (see details) to

use. Types: 'Saddlepoint', 'Normal', 'Gamma', 'InvGamma' and 'Beta' are

supported (default = 'Saddlepoint').

Trunc Vector of length 2 containing the cumulant truncation order and the density trun-

cation order respectively. May take on values 4, 6 and 8 with the constraint that

Trunc[1] >= Trunc[2]. Default is c(4,4).

P Normalization parameter indicating the number of points to use when normaliz-

ing members of the Pearson system (see details)

alpha Normalization parameter controlig the mesh concentration when normalizing

members of the Pearson system (see details). Increasing alpha decreases con-

centration around the mean and vice versa (default alpha = 0).

lower, upper Lower and upper bounds for the normalization range.

Tag can be used to name (tag) an MCMC run e.g. Tag='Run\_1'

wrt If TRUE a .cpp file will be written to the current directory. For bug report diag-

nostics.

#### Value

opt The output from optim.

model.info A list of variables pertaining to inference calculations.

model.info\$elapsed.time

The run-time, in h/m/s format,of the MCMC procedure (excluding compile time).

model.info\$time.homogeneous

'No' if the model has time-homogeneous coefficients and 'Yes' otherwise.

model.info\$p The dimension of theta.

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#### Syntactical jargon

**Synt.** [1]: The coefficients of the 2D GQD may be parameterized using the reserved variable theta. For example:

```
a00 <- function(t){theta[1]*(theta[2]+sin(2*pi*(t-theta[3])))}.
```

**Synt.** [2]: Due to syntactical differences between R and C++ special functions have to be used when terms that depend on t. When the function cannot be separated in to terms that contain a single t, the prod(a,b) function must be used. For example:

```
a00 \leftarrow function(t)\{0.1*(10+0.2*sin(2*pi*t)+0.3*prod(sqrt(t),1+cos(3*pi*t)))\}.
```

Here sqrt(t)\*cos(3\*pi\*t) constitutes the product of two terms that cannot be written i.t.o. a single t. To circumvent this isue, one may use the prod(a,b) function.

**Synt.** [3]: Similarly, the  $^{\wedge}$  - operator is not overloaded in C++. Instead the pow(x,p) function may be used to calculate  $x^{p}$ . For example  $\sin(2*pi*t)^{3}$  in:

```
a00 \leftarrow function(t)\{0.1*(10+0.2*pow(sin(2*pi*t),3))\}.
```

#### Warning

Warning [1]: The parameter mesh is used to discretize the transition horizons between successive observations. It is thus important to ensure that mesh is not too small when large time differences are present in time. Check output for max(dt) and divide by mesh.

**Warning [2]:** Note that minus the likelihood is minimized, as such the optim output (hessian) needs to be adjusted accordingly if used for calculating confidence intervals. Furthermore, GQD.mle may be temperamental under certain conditions

# Author(s)

Etienne A.D. Pienaar: <etiennead@gmail.com>

#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

Daniels, H.E. 1954 Saddlepoint approximations in statistics. Ann. Math. Stat., 25:631-650.

Eddelbuettel, D. and Romain, F. 2011 Rcpp: Seamless R and C++ integration. *Journal of Statistical Software*, **40**(8):1–18,. URL http://www.jstatsoft.org/v40/i08/.

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Varughese, M.M. 2013 Parameter estimation for multivariate diffusion systems. *Comput. Stat. Data An.*, **57**:417–428.

# See Also

```
GQD.remove, GQD.mcmc, BiGQD.mcmc, BiGQD.mle, GQD.passage and GQD.TIpassage.
```

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#### **Examples**

```
# Simulate a time inhomogeneous diffusion.
  data(SDEsim1)
  attach(SDEsim1)
  par(mfrow=c(1,1))
  \texttt{expr1} = \texttt{expression}(\texttt{dX[t]} = \texttt{2} \times \texttt{X[t]} \times (5 + 3 \times \sin(0.5 \times \text{pi} \times \text{t}) - \texttt{X[t]}) \times \texttt{dt} + 0.5 \times \texttt{X[t]} \times \texttt{dW[t]})
  plot(Xt^*time,type='l',col='blue',xlab='Time~(t)',ylab=expression(X[t]),main=expr1)
 # Define coefficients of the process.
  G0 \leftarrow function(t)\{theta[1]*(theta[2]+theta[3]*sin(0.25*pi*t))\}
  G1 <- function(t){-theta[1]}</pre>
  Q0 \leftarrow function(t){theta[4]*theta[4]}
                                                             # Starting values for the chain
  theta.start <-c(1,1,1,1)
                                                             # Number of mesh points
  mesh.points <- 10
  m1 <- GQD.mle(Xt,time,mesh=mesh.points,theta=theta.start)</pre>
  G1 <- function(t){theta[1]*(theta[2]+theta[3]*sin(0.25*pi*t))}
  G2 <- function(t){-theta[1]}</pre>
  Q2 \leftarrow function(t)\{theta[4]*theta[4]\}
  theta.start <-c(1,1,1,1)
                                                             # Starting values for the chain
  mesh.points <- 10
                                                             # Number of mesh points
  m2 <- GQD.mle(Xt,time,mesh=mesh.points,theta=theta.start)</pre>
  # Check estimates:
  GQD.estimates(m1)
  GQD.estimates(m2)
  # Compare models:
  GQD.aic(list(m1,m2))
```

GQD.passage

Calculate the First Passage Time Density of a Time-Homogeneous GQD Process to a Fixed Barrier.

# **Description**

GQD.passage uses the cumulant truncation procedure of Varughese (2013) in conjunction with a Volterra-type integral equation developed by Buonocore et al. (1987) in order to approximate the

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first passage time density of a time-homogeneous univariate GQD

$$dX_t = (theta[1] + theta[2]X_t + theta[3]X_t^2)dt + \sqrt{theta[4] + theta[5]X_t + theta[6]X_t^2}dW_t,$$
 to a fixed barrier.

## Usage

```
GQD.passage(Xs, B, theta, t, delt)
```

### **Arguments**

Xs Initial value of the process.

B Fixed barrier (>Xs).

theta Parameter vector giving the coefficients of the time-homogeneous GQD.

The time horizon up to and including which the density is to be evaluated.

delt Stepsize for the solution of the first passage time density.

#### Value

density The approximate first passage time density.

time The time points at which the approximation is evaluated.

prob.coverage The approximate cumulative probability coverage.

#### Warning

**Warning** [1]: Some instability may occur when delt is large or where the saddlepoint approximation fails. As allways it is important to check both the validity of the diffusion process under the given parameters and the quality of the sadlepoint approximation. For a given set of parameters the latter can be checked using GQD.density.

**Warning [2]**: The first passage time problem is considered from one side only i.e. Xs<B. For Xs>B one may equivalently consider Yt=-X\_t, apply Ito's lemma and proceed as above.

#### Note

**Note** [1]: Since time-homogeneity is assumed for the present implementation, the interface of GQD.mcmc etc. is discarded and the model is inferred from the non-zero values of theta. For example theta =  $c(0.5*10, -0.5, 0, 0.5^2, 0, 0)$  defines an Ornstein-Uhlenbeck model.

# Author(s)

Etienne A.D. Pienaar: <etiannead@gmail.com>

# References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

A. Buonocore, A. Nobile, and L. Ricciardi. 1987 A new integral equation for the evaluation of first-passage- time probability densities. *Adv. Appl. Probab.* **19**:784–800.

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Eddelbuettel, D. and Sanderson, C. 2014 Repparmadillo: Accelerating r with high-performance C++ linear algebra. *Computational Statistics and Data Analysis*, **71**:1054–1063. URL http://dx.doi.org/10.1016/j.csda.2013.02.005.

Feagin, T. 2007 A tenth-order Runge-Kutta method with error estimate. *In Proceedings of the IAENG Conf. on Scientific Computing*.

R. G. Jaimez, P. R. Roman and F. T. Ruiz. 1995 A note on the volterra integral equation for the first-passage-time probability density. *Journal of applied probability*, 635–648.

Varughese, M.M. 2013 Parameter estimation for multivariate diffusion systems. *Comput. Stat. Data An.*, **57**:417–428.

#### See Also

GQD. density for functions that generate the transitional density of GQDs. GQD. mcmc and GQD. remove for MCMC procedures to perform inference on GQDs.

```
# Calculate the first passage time from state X_0 = 7 to X_T = 10 for
# various diffusions, with T the first passage time.
 res1 <- GQD.passage(7,10,c(0.1*10,-0.1,0,0.2,0,0),25,1/100)
 res2 <- GQD.passage(7,10,c(0.1*10,-0.1,0,0,0.2,0),25,1/100)
 res3 <- GQD.passage(7,10,c(0,0.1*10,-0.1,0.5^2,0,0),25,1/100)
 res4 <- GQD.passage(7,10,c(0,0.1*10,-0.1,0,0,0.1*2),25,1/100)
 expr1 <- expression(dX[t]==(1-0.1*X[t])*dt+sqrt(0.2)*dW[t])
 expr2 <- expression(dX[t]==(1-0.1*X[t])*dt+sqrt(0.2*X[t])*dW[t])
 expr3 <- expression(dX[t]==(1*X[t]-0.1*X[t]^2)*dt+0.5*dW[t])
 expr4 \leftarrow expression(dX[t]==(1*X[t]-0.1*X[t]^2)*dt+0.1*X[t]*dW[t])
# Plot the resulting first passage time densities.
#-----
 par(mfrow=c(2,2))
 plot(res1$density~res1$time,type='l',main=expr1,xlab='Time (t)',ylab='density',col='blue')
 plot(res2$density~res2$time,type='1',main=expr2,xlab='Time (t)',ylab='density',col='blue')
 plot(res3$density~res3$time,type='1',main=expr3,xlab='Time (t)',ylab='density',col='blue')
 plot(res4$density~res4$time,type='1',main=expr4,xlab='Time (t)',ylab='density',col='blue')
```

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Quick Plots for DiffusionRgqd Objects

## **Description**

GQD.plot() recognizes output objects calculated using routines from the **DiffusionRgqd** package and subsequently constructs an appropriate plot, for example a perspective plot of a transition density.

# Usage

```
GQD.plot(x, thin = 1, burns, h = FALSE)
```

## **Arguments**

x Generic GQD-objects, i.e. res = GQD.density().

thin Thinning interval for .mcmc objects.

burns Number of parameter draws to discard for .mcmc objects.

h if TRUE a histogram is drawn i.s.o. a trace plot.

#### Value

Varies in accordance with input type.

#### Author(s)

```
Etienne A.D. Pienaar: <etiannead@gmail.com>
```

#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

## See Also

```
GQD.mcmc, GQD.mle, GQD.density, BiGQD.density etc.
```

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```
Tmax <- 5  # Time horizon
Tstart <- 1  # Time starts at 1
increment <- 1/100  # Incremental time steps

# Generate the transitional density
M <- GQD.density(Xs=initial,Xt=states,s=Tstart,t=Tmax,delt=increment)

GQD.plot(M)</pre>
```

GQD.remove

Remove the Coefficients of a GQD Model.

# **Description**

Removes any existing coefficient functions from the current workspace.

# Usage

```
GQD.remove()
```

#### **Details**

GQD. remove clears the workspace of functions with names that match the coefficients of the 1D GQD. This may be used when more than one model is specified in a given session.

# Value

No value is returned.

## Note

GQD. remove simply searches the workspace for functions with definitions that match the form of the DiffusionRgqd interface and removes them from the workspace, freeing up the user to redefine a diffusion with new coefficients.

# Author(s)

```
Etienne A.D. Pienaar: <etiennead@gmail.com>
```

#### References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

# See Also

```
GQD. density and BiGQD. density.
```

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GQD.TIpassage	Compute the First Passage Time Density of a GQD With Time Inho-
	mogeneous Coefficients.

# **Description**

GQD.TIpassage() solves first passage time problems for GQDs with time dependent coefficients:

$$dX_t = (G_0(t) + G_1(t)X_t + G_2(t)X_t^2)dt + \sqrt{Q_0(t) + Q_1(t)X_t + Q_2(t)X_t^2}dW_t$$

to a fixed barrier. The function combines the cumulant truncation procedure of Varughese (2013) with a numerical solution to a non-singular Volterra integral equation for the first passage time density, developed by Buonocore et al. (1987), in order to generate an approximate solution.

# Usage

```
GQD.TIpassage(Xs,B, s, t, delt, theta=c(0), IEQ.type='Buonocore', wrt=FALSE)
```

# **Arguments**

Xs	Initial value of the diffusion process at time tmin.
В	Fixed barrier (or first constant in static barier transform - see detail [1]).
S	Starting time for the diffusion process (see detail [2]).
t	The time horizon up to and including which the density is to be evaluated.
delt	Stepsize for the solution of the first passage time density.
theta	Parameter vector for parameters contained in the coefficients (if required).
IEQ.type	Currently only IEQ.type = "Buonocore" is supported.
wrt	If TRUE a .cpp file will be written to the current directory. For bug report diagnostics.

# **Details**

Detail [1]: First passage throug a time dependant barrier may be analised by applying the transform:

$$Y_t = X_t - B_t,$$

if  $B_t$  may can be decomposed as

$$B_t = k + f(t).$$

By applying Ito's lemma the revised drift and diffusion functionals, and first passage parameters may be inferred.

**Detail** [2]: The starting time is of particular importance when the drift and/or diffusion terms are time-inhomogeneous. Take care to select the correct starting time - especially if the drift or diffusion components which are time dependant have poles or singular points in the time domain.

## Value

density The approximate first passage time density.

time The time points at which the approximation is evaluated. prob.coverage The approximate cumulative probability coverage.

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#### Warning

**Warning [1]:** Some instability may occur when delt is large or where the saddlepoint approximation fails. As allways it is important to check both the validity of the diffusion process under the given parameters and the quality of the saddlepoint approximation. For a given set of parameters the latter can be checked using GOD. density.

**Warning [2]:** The first passage time problem is considered from one side only i.e. Xs<B. For Xs>B one may equivalently consider Yt=-X\_t, apply Ito's lemma and proceed as above.

#### Note

**Note** [1]: The coefficients od the GQD may be parameterized using the reserved variable theta. For example:

```
G0 <- function(t){theta[1]*(theta[2]+sin(2*pi*(t-theta[3])))}</pre>
```

may be used so long as values are asigned in the function call, say

```
GQD.TIpassage(Xs=3,B=11,tmin=1,tmax=10,delt=1/100,theta=c(1,10,0.5)).
```

**Note** [2]: Due to syntactical differences between R and C++ special functions have to be used when terms that depend on t. When the function cannot be separated in to terms that contain a single t, the prod(a,b) function must be used. For example (see examples below):

```
GO \leftarrow function(t)\{0.1*(10+0.2*sin(2*pi*t)+0.3*prod(sqrt(t),1+cos(3*pi*t)))\}.
```

Here sqrt(t)\*cos(3\*pi\*t) constitutes the product of two terms that cannot be written i.t.o. a single t. To circumvent this isue, one may use the prod(a,b) function.

**Note** [3]: Similarly, the  $^{\land}$  - operator is not overloaded in C++. Instead the pow(x,p) function may be used to calculate  $x^{\land}p$ . For example  $\sin(2*pi*t)^{\land}3$  in:

```
G0 <- function(t)\{0.1*(10+0.2*pow(sin(2*pi*t),3))\}.
```

**Note [4]:** delt is used as the stepsize of the Runge-Kutta method used to numerically solve a system of ODEs used to approximate the cumulants of the underlying diffusion procees. The 10th-order scheme of Feagin (2007) is used as the default method.

## Author(s)

Etienne A.D. Pienaar: <etiennead@gmail.com>

## References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

A. Buonocore, A. Nobile, and L. Ricciardi. 1987 A new integral equation for the evaluation of first-passage- time probability densities. *Adv. Appl. Probab.* **19**:784–800.

Daniels, H.E. 1954 Saddlepoint approximations in statistics. Ann. Math. Stat., 25:631–650.

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#### See Also

GQD. density for functions that generate the transitional density of GQDs and GQD. mcmc for MCMC procedures for GQD models.

```
# Generate the first passage time density of a CIR process with time
# dependant drift to a fixed barrier.
 # Remove any existing coefficients.
 GQD.remove()
 # Define the coefficients of the process.
 G0 \leftarrow function(t)\{10+0.5*sin(2*pi*t)\}
 G1 \leftarrow function(t)\{-1\}
 Q1 \leftarrow function(t)\{0.25\}
 #Define the parameters of the first passage time problem.
 delt <- 1/100  # The stepsize for the solution
 X0 <- 8
                      # The initial value of the process
 BB <- 11
                      # Fixed barrier
 T0 <- 2
                      # Starting time of the diffusion
 TT <- 10
                       # Time horizon of the computation
 # Run the calculation
 res1 <- GQD.TIpassage(X0,BB,T0,TT,delt)</pre>
 # Remove any existing coefficients.
 GQD.remove()
 # Redefine the coefficients.
 G0 <- function(t){ 0.1*(10+0.2*sin(2*pi*t)+0.3*prod(sqrt(t),1+cos(3*pi*t)))}
 G1 \leftarrow function(t)\{-0.1*(1+0.2*sin(2*pi*t))\}
 Q1 \leftarrow function(t)\{0.25\}
 # Redefine the parameters of the f.p.t. problem.
 delt <- 1/100
 X0 <- 8
 BB <- 11
 T0 <- 1
 TT <- 10
 # Run the calculation
 res2 <- GQD.TIpassage(X0,BB,T0,TT,delt)</pre>
```

```
# Plot the two solutions.
expr1 <- expression(dX[t]==(10+0.5*sin(2*pi*t)-X[t])*dt+0.25*sqrt(X[t])*dW[t])
 \exp r^2 \leftarrow \exp ression(dX[t] == (0.1*(10+0.2*sin(2*pi*t)+0.3*sqrt(t)*(1+cos(3*pi*t)))
                   -0.1*(1+0.2*sin(2*pi*t))*X[t])*dt+0.25*sqrt(X[t])*dW[t]))
 par(mfrow=c(1,1))
 plot(res1$density~res1$time,type='l',col='blue',
      ylab='Density',xlab='Time',main=expr1,cex.main=0.95)
 plot(res2$density~res2$time,type='1',col='red',
      ylab='Density',xlab='Time',main =expr2,cex.main=0.95)
# Let's see how sensitive the first passage density is w.r.t a speed parameter
# of a non-linear diffusion.
GQD.remove()
# Redefine the coefficients with a parameter theta:
G1 \leftarrow function(t)\{theta[1]*(10+0.2*sin(2*pi*t)+0.3*prod(sqrt(t),1+cos(3*pi*t)))\}
G2 <- function(t){-theta[1]}</pre>
Q2 \leftarrow function(t)\{0.1\}
# Now just give a value for the parameter in the standard fashion:
res3=GQD.TIpassage(8,12,1,4,1/100,theta=c(0.5))
plot(res3$density~res3$time,type='1',col=2,ylim=c(0,1.0),
main='First Passage Time Density',ylab='Density',xlab='Time',cex.main=0.95)
# Change the parameter and see the effect on the f.p.t. density.
th.seq=seq(0.1, 0.5, 1/20)
for(i in 2:length(th.seq))
 res3=GQD.TIpassage(8,12,1,4,1/100,,theta=c(th.seq[i]))
 lines(res3$density~res3$time,type='l',col=rainbow(10)[i])
lines(res3$density~res3$time,type='l',col=rainbow(10)[i],lwd=2)
legend('topright',legend=th.seq,col=rainbow(10),lty='solid',cex=0.75,
title=expression(theta[1]))
```

RcppArmadillo-Functions

A Junk Funktion For Build Purposes

# **Description**

This function was created as a filler in order for the package to build correctly.

## Usage

```
junkfunction()
```

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#### **Details**

This function was created as a filler in order for the package to build correctly.

#### Value

junkfunction() does nothing useful.

#### Author(s)

Etienne A.D. Pienaar

#### References

See the documentation for Armadillo, and RcppArmadillo, for more details.

SDEsim1

A Simulated Diffusion with Sinusoidal Drift and State-Dependant Diffusion Coefficient.

#### **Description**

The dataset contains discretely sampled observations for a simulated stochastic differential equation (SDE) with dynamics:

$$dX_t = 2X_t(5 + 3\sin(0.25\pi t) - X_t)dt + 0.5X_t dW_t$$

where  $dW_t$  is standard Brownian motion, t is time and  $X_0 = 7$ .

## Usage

data(SDEsim1)

## Format

A data frame with 401 observations with the following variables:

- 1. Xt: A numeric vector of simulated observations.
- 2. time: A numeric vector of time nodes at which Xt was observed (time[i+1]-time[i] = 1/4).

# **Details**

The process was simulated by numerically solving the SDE using a Euler-Maruyama scheme with stepsize = 1/2000. Subsequently each 200-th observation was recorded in order to construct the resulting time series.

## Author(s)

Etienne A.D. Pienaar: <etiannead@gmail.com>

## References

Updates available on GitHub at https://github.com/eta21. Visit http://etiennead.wix.com/diffusionr for more details on the DiffusionRgqd package.

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#### **Examples**

```
data(SDEsim1)
attach(SDEsim1)
par(mfrow=c(1,1))
expr1=expression(dX[t]==2*X[t]*(5+3*sin(0.5*pi*t)-X[t])*dt+0.5*X[t]*dW[t])
plot(Xt~time,type='l',col='blue',xlab='Time (t)',ylab=expression(X[t]),main=expr1)
```

SDEsim2

A Simulated Non-Linear Bivariate Diffusion

## **Description**

The dataset contains discretely sampled observations for a simulated stochastic differential equation (SDE) with dynamics:

$$dX_{t} = 2.0(Y_{t} - X_{t})dt + 0.3\sqrt{X_{t}Y_{t}}dW_{t}$$
$$dY_{t} = 1.0(5 - Y_{t})dt + 0.5\sqrt{Y_{t}}dB_{t}$$

where dW\_t and dB\_t are standard Brownian motions, t is time and  $X_0 = 5$ ,  $Y_0 = 5$ .

## Usage

```
data("SDEsim2")
```

#### **Format**

A data frame with 801 observations on the following 3 variables.

Xt Xt trajectory of the diffusion.

Yt Yt trajectory of the diffusion.

time Time vector (time[i+1]-time[i] = 1/8).

#### **Details**

For a full analysis of this dataset check out Example 7.5 in the example scripts at https://github.com/eta21/DiffusionRgqd-Downloads.

SDEsim3

SDEsim3

Simulated Stochastic Lotka-Volterra Eqns

# **Description**

The dataset contains discretely sampled observations for a simulated stochastic differential equation (SDE) with dynamics:

$$dX_t = (1.5X_t - 0.4X_tY_t)dt + \sqrt{0.05X_t}dW_t$$
  
$$dY_t = (-1.5Y_t + 0.4X_tY_t - 0.2Y_t^2)dt + \sqrt{0.1X_t}dB_t$$

where dW\_t and dB\_t are standard Brownian motions, t is time and  $X_0 = 5$ ,  $Y_0 = 5$ .

# Usage

data("SDEsim3")

#### **Format**

A data frame with 1001 observations on the following 3 variables.

time A numeric vector of time nodes at which means are calculated (time[i+1]-time[i] = 1/4). mx Mean Xt trajectory of the diffusion.

my Mean Yt trajectory of the diffusion.

SDEsim4

A Simulated Non-Linear Bivariate Diffusion With Time-Inhomogeneous Coefficients

# Description

The dataset contains discretely sampled observations for a simulated stochastic differential equation (SDE) with dynamics:

$$dX_t = (1.0(7.5 - X_t) + 1.5Y_t)dt + 0.5\sqrt{X_tY_t}dW_t$$
$$dY_t = (1.5(5 - Y_t) + 3\sin(0.25\pi t))dt + 0.25\sqrt{Y_t}dB_t$$

where dW\_t and dB\_t are standard Brownian motions, t is time and  $X_0 = 10$ ,  $Y_0 = 5$ .

# Usage

data("SDEsim4")

#### **Format**

A data frame with 401 observations on the following 3 variables.

Xt Xt trajectory of the diffusion.

Yt Yt trajectory of the diffusion.

time Time vector.

40 SDEsim4

# **Details**

For a full analysis of this dataset check out Example 7.5 in the example scripts at https://github.com/eta21/DiffusionRgqd-Downloads.

```
data(SDEsim4)
data(SDEsim4)
attach(SDEsim4)
# Have a look at the time series:
plot(Xt~time,type='l',col='blue',ylim=c(0,25),main='Simulated Data',
xlab='Time (t)',ylab='State',axes=FALSE)
lines(Yt~time,col='red')
axis(1,seq(0,100,5))
axis(1,seq(0,100,5/10),tcl=-0.2,labels=NA)
axis(2,seq(0,25,2))
axis(2,seq(0,25,2/10),tcl=-0.2,labels=NA)
```

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